AMENDMENTS TO THE CLAIMS

Cancel Claims 6-11.

Please add new Claims 12 and 13.

12. (New) A method for identifying at least one stable docking configuration of heteroatoms in a ligand with a biopolymer comprising:

A. inputting the three-dimensional coordinates for a biopolymer and a ligand in a conformation,

B. setting dummy atoms at the positions of heteroatoms that can be hydrogen-bonded with the hydrogen bonding groups in the biopolymer,

C. comparing the distances between the dummy atoms and hoteroatoms while changing conformations of said ligand, and

D. selecting a configuration of the heteroatoms in the ligand that corresponds with the configuration of the dummy atoms.

D1

13. (New) A method for estimating the active conformation of a ligand with a biopolymer comprising:

A. inputting the three-dimensional coordinates for a biopolymer and a ligand in a conformation,

B. setting dummy atoms at the positions of heteroatoms that can be hydrogen-bonded with the hydrogen bonding groups in the biopolymer,

C. comparing the distances between the dummy atoms and heteroatoms while changing conformations of said ligand,

D. selecting a configuration of the heteroatoms in the ligand that corresponds with the configuration of the dummy atoms, and

D1 cont'd E. estimating at least one stable docking structure between said biopolymer and said ligand.